Assessing the Effectiveness of Acceleration Methods for Deterministic Neutron Transport Solvers Building a new tool for developers.

J. S. Rehak



ANS Summer Meeting: Acceleration Methods

June 10th, 2020



A majority of our limited time and effort (and funding) should be dedicated to designing new and better acceleration methods, **not implementing and analyzing results**.

Outline

- 1 Why acceleration methods?
- 2 Analysis and implementation challenges
- 3 Design paradigm
- Status and future work

Steady-state Boltzman Transport Equation

Our problem of interest is the time-independent transport equation on a domain of interest $\vec{r} \in V$ [3],

$$\begin{split} \left[\hat{\Omega} \cdot \nabla + \Sigma_t(\vec{r}, E) \right] \psi(\vec{r}, E, \hat{\Omega}) \\ &= \int_0^\infty dE' \int_{4\pi} d\hat{\Omega}' \Sigma_s(\vec{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega}) \psi(\vec{r}, E', \hat{\Omega}') \\ &+ Q(\vec{r}, E, \hat{\Omega}) \;, \end{split}$$

with a given boundary condition,

$$\psi(\vec{r}, E, \hat{\Omega}) = \Gamma(\vec{r}, E, \hat{\Omega}), \quad \vec{r} \in \partial V, \quad \hat{\Omega} \cdot \hat{n} < 0$$

◆ロト ◆部 → ◆恵 → 恵 ・ りへで

J.S. Rehak BART June 10th, 2020 1/19

Discretizations:

• Split up the spatial domain into cells.

Discretizations:

- Split up the spatial domain into cells.
- Split up the energy domain into groups (multi-group equations).

Discretizations:

- Split up the spatial domain into cells.
- Split up the energy domain into groups (multi-group equations).
- Solve along particular angles (collocation).

Discretizations:

- Split up the spatial domain into cells.
- Split up the energy domain into groups (multi-group equations).
- Solve along particular angles (collocation).

$$\mathbf{L}\vec{\Psi} = \mathbf{M}\left[\mathbf{S} + \frac{1}{k}\mathbf{F}\right]\vec{\Phi}$$

Discretizations:

- Split up the spatial domain into cells.
- Split up the energy domain into groups (multi-group equations).
- Solve along particular angles (collocation).

$$\mathbf{L}\vec{\Psi} = \mathbf{M} \left[\mathbf{S} + \frac{1}{k} \mathbf{F} \right] \vec{\Phi}$$

(Scattering) source iteration $\vec{\Psi}_{(k+1)} = \mathbf{L}^{-1}\mathbf{M}\left[\mathbf{S}\vec{\Phi}_{(k)} + \frac{1}{k}\mathbf{F}\vec{\Phi}_{(0)}\right]$

Power iteration $\vec{\Psi}_{(k+1)} = \mathbf{L}^{-1} \mathbf{M} \left[\mathbf{S} \vec{\Phi}_{(0)} + \tfrac{1}{k} \mathbf{F} \vec{\Phi}_{(k)} \right]$

◆ロト ◆部ト ◆重ト ◆重ト ■ からぐ

J.S. Rehak BART June 10th, 2020 2/19

Design paradigm

Why acceleration methods?

00000

Convergence of Source Iteration

Gauss-Seidel source iteration can converge arbitrarily slowly as Σ_s/Σ_t approaches unity.

Design paradigm

Convergence challenges

Convergence of Source Iteration

Gauss-Seidel source iteration can converge arbitrarily slowly as Σ_s/Σ_t approaches unity.

Convergence of Power Iteration

Power iteration can converge arbitrarily slowly as the dominance ratio k_1/k_0 approaches unity.

Convergence challenges

Convergence of Source Iteration

Gauss-Seidel source iteration can converge arbitrarily slowly as Σ_s/Σ_t approaches unity.

Convergence of Power Iteration

Power iteration can converge arbitrarily slowly as the dominance ratio k_1/k_0 approaches unity.

Motivates the development of **acceleration methods** to address these issues.

- Source Iteration: Diffusion two-grid method (TG).
- Power Iteration: Nonlinear diffusion acceleration (NDA).

4 D > 4 A > 4 B > 4 B > B = 900

Primary goal

To reduce the total amount of computational work required for an iterative method to converge[1].

Primary goal

To reduce the total amount of computational work required for an iterative method to converge[1].

The error in step ℓ , is given by

$$\vec{e}_{(\ell)} = \vec{\Psi}^* - \vec{\Psi}_{(\ell)} \ . \label{eq:elliptic_elliptic}$$

Primary goal

To reduce the total amount of computational work required for an iterative method to converge[1].

The error in step ℓ , is given by

$$\vec{e}_{(\ell)} = \vec{\Psi}^* - \vec{\Psi}_{(\ell)} \ . \label{eq:epsilon}$$

Our method converges in N steps when

$$\left\| \vec{e}_{(N)} \right\| < \varepsilon \;,$$

Primary goal

To reduce the total amount of computational work required for an iterative method to converge[1].

The error in step ℓ , is given by

$$\vec{e}_{(\ell)} = \vec{\Psi}^* - \vec{\Psi}_{(\ell)} .$$

Our method converges in N steps when

$$\left\| \vec{e}_{(N)} \right\| < \varepsilon \;,$$

with total computational work

$$W = \sum_{\ell=1}^{N} w_{(\ell)} .$$

4 D > 4 A > 4 E > 4 E > 9 Q Q

J.S. Rehak BART

An accelerated method seeks to reduce the total computational work to achieve the same convergence. It is effective if

$$\sum_{\ell=1}^{N'} w'_{(\ell)} < \sum_{\ell=1}^{N} w_{(\ell)}$$

An accelerated method seeks to reduce the total computational work to achieve the same convergence. It is effective if

$$\sum_{\ell=1}^{N'} w'_{(\ell)} < \sum_{\ell=1}^{N} w_{(\ell)}$$

Why acceleration methods?

We can (and must) remove the same amount of error to achieve convergence using less (or a finite amount) of computational work.

June 10th, 2020

Outline

- Why acceleration methods?
- 2 Analysis and implementation challenges
- Oesign paradigm
- **4** Status and future work

Challenge

We need to modify an existing code, or create a new code to test our acceleration method.

Challenge

We need to modify an existing code, or create a new code to test our acceleration method.

Production codes can be difficult to modify.

Challenge

We need to modify an existing code, or create a new code to test our acceleration method.

- Production codes can be difficult to modify.
- Writing new codes can be time consuming and costly.

Challenge

We need to modify an existing code, or create a new code to test our acceleration method.

- Production codes can be difficult to modify.
- Writing new codes can be time consuming and costly.
- Reproducibility and testing is difficult.

Challenge

We need to modify an existing code, or create a new code to test our acceleration method.

- Production codes can be difficult to modify.
- Writing new codes can be time consuming and costly.
- Reproducibility and testing is difficult.

Challenge

We need to modify an existing code, or create a new code to test our acceleration method.

- Production codes can be difficult to modify.
- Writing new codes can be time consuming and costly.
- · Reproducibility and testing is difficult.

What do we need?

A coding framework designed with the developer end-user in mind, that is portable and reproducible.

Defining work

Defining work

In general, we use inversions of the transport matrix – explicitly or implicitly (sweeps) – as a unit of work.

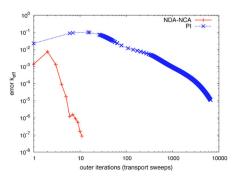


Figure 1: NDA convergence vs standard power iteration [7]

Challenge

Work definition requires (good) assumptions about algorithm efficiency.

Challenge

Work definition requires (good) assumptions about algorithm efficiency.

$$\sum_{\ell=1}^{N'} w'_{(\ell)} < \sum_{\ell=1}^{N} w_{(\ell)}$$

Challenge

Work definition requires (good) assumptions about algorithm efficiency.

$$\sum_{\ell=1}^{N'} w'_{(\ell)} < \sum_{\ell=1}^{N} w_{(\ell)}$$

$$w_{(\ell)} = w_{(\text{inv})} + w_{(\text{other})} \approx w_{(\text{inv})}$$

Challenge

Work definition requires (good) assumptions about algorithm efficiency.

$$\begin{split} \sum_{\ell=1}^{N'} w'_{(\ell)} < \sum_{\ell=1}^{N} w_{(\ell)} \\ w_{(\ell)} &= w_{(\mathsf{inv})} + w_{(\mathsf{other})} \approx w_{(\mathsf{inv})} \\ N'w'_{(\mathsf{inv})} < Nw_{(\mathsf{inv})} \end{split}$$

Challenge

Work definition requires (good) assumptions about algorithm efficiency.

$$\sum_{\ell=1}^{N'} w'_{(\ell)} < \sum_{\ell=1}^{N} w_{(\ell)}$$

$$w_{(\ell)} = w_{(\text{inv})} + w_{(\text{other})} \approx w_{(\text{inv})}$$

$$N'w'_{(\mathsf{inv})} < Nw_{(\mathsf{inv})}$$

Relying on the number of sweeps as a measure of effectiveness relies on $w'_{(\text{inv})} \approx w_{(\text{inv})}.$

<ロ > < 回 > < 回 > < 巨 > < 巨 > 三 の < (で

J.S. Rehak BART

Analysis challenges

Challenge

Work definition requires (good) assumptions about algorithm efficiency.

$$\sum_{\ell=1}^{N'} w'_{(\ell)} < \sum_{\ell=1}^{N} w_{(\ell)}$$

$$w_{(\ell)} = w_{(\text{inv})} + w_{(\text{other})} \approx w_{(\text{inv})}$$

$$N'w'_{(\mathsf{inv})} < Nw_{(\mathsf{inv})}$$

Relying on the number of sweeps as a measure of effectiveness relies on $w'_{(\text{inv})} \approx w_{(\text{inv})}.$

This becomes complicated as our acceleration methods become more complex, and take on more work.

J.S. Rehak BART June 10th, 2020 8/19

Challenge

We want to validate why our methods work.

J.S. Rehak BART

Challenge

We want to validate why our methods work.

 The methods we develop are backed up by math and our understanding of the problem.

Challenge

We want to validate why our methods work.

- The methods we develop are backed up by math and our understanding of the problem.
- If a method is successful in accelerating a solve, it's not always clear why.

Challenge

We want to validate why our methods work.

- The methods we develop are backed up by math and our understanding of the problem.
- If a method is successful in accelerating a solve, it's not always clear why.
- Combinations of methods may make the mathematical analysis difficult or impossible.

Challenge

We want to validate why our methods work.

- The methods we develop are backed up by math and our understanding of the problem.
- If a method is successful in accelerating a solve, it's not always clear why.
- Combinations of methods may make the mathematical analysis difficult or impossible.

Challenge

We want to validate why our methods work.

- The methods we develop are backed up by math and our understanding of the problem.
- If a method is successful in accelerating a solve, it's not always clear why.
- Combinations of methods may make the mathematical analysis difficult or impossible.

What do we need?

Additional, good data that enables us to assess the effectiveness of our method.

J.S. Rehak BART June 10th, 2020

Analysis Challenges

A few challenges when analyzing the effectiveness of acceleration schemes include:

Work definition requires assumptions about algorithm efficiency.

10 / 19

Design paradigm

Analysis Challenges

A few challenges when analyzing the effectiveness of acceleration schemes include:

- Work definition requires assumptions about algorithm efficiency.
- We need good data to show us why our methods are working.

BART

Analysis Challenges

A few challenges when analyzing the effectiveness of acceleration schemes include:

- Work definition requires assumptions about algorithm efficiency.
- We need good data to show us why our methods are working.
- Combined or complex schemes may invalidate assumptions.

Analysis Challenges

A few challenges when analyzing the effectiveness of acceleration schemes include:

- Work definition requires assumptions about algorithm efficiency.
- We need good data to show us why our methods are working.
- Combined or complex schemes may invalidate assumptions.
- Implementation and reproducibility can be difficult.

Outline

- Why acceleration methods?
- Analysis and implementation challenges
- Obesign paradigm
- **4** Status and future work

The Bay Area Radiation Transport (BART) is motivated by three major design goals. To create a code that,

The Bay Area Radiation Transport (BART) is motivated by three major design goals. To create a code that,

 relieves some of the burden of implementing a novel acceleration method,

The Bay Area Radiation Transport (BART) is motivated by three major design goals. To create a code that,

- relieves some of the burden of implementing a novel acceleration method,
- 2 provides a controlled environment for measuring the effectiveness of the novel method, and,

The Bay Area Radiation Transport (BART) is motivated by three major design goals. To create a code that,

- 1 relieves some of the burden of implementing a novel acceleration method.
- 2 provides a controlled environment for measuring the effectiveness of the novel method, and,
- 3 provides tools for verifying the basis for effectiveness.

J.Ş. Rehak BART

Goal 1

Relieving some of the burden of implementing a novel acceleration method.

Goal 1

Why acceleration methods?

Relieving some of the burden of implementing a novel acceleration method.

BART is designed to be a code focused on a **developer** end-user.

Goal 1

Relieving some of the burden of implementing a novel acceleration method.

BART is designed to be a code focused on a developer end-user.

 Focus on clarity of structure instead of performance (optimization for modification).

Goal 1

Relieving some of the burden of implementing a novel acceleration method.

BART is designed to be a code focused on a developer end-user.

- Focus on clarity of structure instead of performance (optimization for modification).
- Heavy usage of polymorphism.

SystemInitializerI

- + Initialize(System&)
- : void

Goal 1

Relieving some of the burden of implementing a novel acceleration method.

BART is designed to be a code focused on a **developer** end-user.

 Focus on clarity of structure instead of performance (optimization for modification).



- Heavy usage of polymorphism.
- Comprehensive testing coverage.

0000000

Goal 2

Why acceleration methods?

Providing a controlled environment for measuring the effectiveness of the novel method.

Controlled testing environment

Goal 2

Providing a controlled environment for measuring the effectiveness of the novel method.

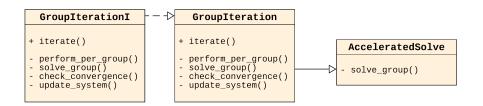
BART is designed to leverage polymorphism to isolate and minimize changes required to implement novel methods.

Controlled testing environment

Goal 2

Providing a controlled environment for measuring the effectiveness of the novel method.

BART is designed to leverage polymorphism to isolate and minimize changes required to implement novel methods.



The use of polymorphism in BART

 Minimizes code changes needed to implement new methods, making it faster and easier.

The use of polymorphism in BART

- Minimizes code changes needed to implement new methods, making it faster and easier.
- Eases comparisons of the accelerated solve to a control solve.

J.S. Rehak BART

The use of polymorphism in BART

- Minimizes code changes needed to implement new methods, making it faster and easier.
- Eases comparisons of the accelerated solve to a control solve.
- Makes the modifications portable.

The use of polymorphism in BART

- Minimizes code changes needed to implement new methods, making it faster and easier.
- Eases comparisons of the accelerated solve to a control solve.
- Makes the modifications *portable*.
- Enables us to compare the implementation of the method to dis-aggregate the computer science from the method itself.

Design paradigm ○○○○○●○

Why acceleration methods?

0000000

Instrumentation

Goal 3

Provide tools for verifying the basis for effectiveness.

Instrumentation

Goal 3

Provide tools for verifying the basis for effectiveness.

BART will include the ability to *instrument* a solve to gather enough data to draw useful conclusions about the effectiveness of acceleration schemes.

Instrumentation

Goal 3

Provide tools for verifying the basis for effectiveness.

BART will include the ability to *instrument* a solve to gather enough data to draw useful conclusions about the effectiveness of acceleration schemes.

- Storage of solve parameters (eigenvalues, fluxes).
- Storage of hierarchy of iterations.
- Calculation and storage of error or residual.
- Analysis of Fourier error modes coefficients.

J.S. Rehak BART June 10th, 2020 15 / 19

Instrumentation

Goal 3

Provide tools for verifying the basis for effectiveness.

BART will include the ability to *instrument* a solve to gather enough data to draw useful conclusions about the effectiveness of acceleration schemes.

- Storage of solve parameters (eigenvalues, fluxes).
- Storage of hierarchy of iterations.
- Calculation and storage of error or residual.
- Analysis of Fourier error modes coefficients.

Important

Adding new instrumentation must be easy!



15 / 19

J.S. Rehak BART June 10th, 2020

Goals Reprise

To create a code that,

- relieves some of the burden of implementing a novel acceleration method,
- 2 provides a controlled environment for measuring the effectiveness of the novel method, and,
- 3 provides tools for verifying the basis for effectiveness.

Goals Reprise

To create a code that,

- relieves some of the burden of implementing a novel acceleration method,
- 2 provides a controlled environment for measuring the effectiveness of the novel method, and,
- 3 provides tools for verifying the basis for effectiveness.

Getting goal three right relies on doing one and two really well.

Outline

- Why acceleration methods?
- Analysis and implementation challenges
- Oesign paradigm
- **4** Status and future work

Design paradigm

The BART Code

Deterministic, finite-element-based transport code.

- Deterministic, finite-element-based transport code.
- Coded in C++, using the C++17 standard. A python script can automate creation of input files.

- Deterministic, finite-element-based transport code.
- Coded in C++, using the C++17 standard. A python script can automate creation of input files.
- Uses the deal.II finite-element library [4].

- Deterministic, finite-element-based transport code.
- Coded in C++, using the C++17 standard. A python script can automate creation of input files.
- Uses the deal.II finite-element library [4].
- Parallel processor (MPI) calculations are supported using PETSc [9, 8, 2].

- Deterministic, finite-element-based transport code.
- Coded in C++, using the C++17 standard. A python script can automate creation of input files.
- Uses the deal.II finite-element library [4].
- Parallel processor (MPI) calculations are supported using PETSc [9, 8, 2].
- Uses the GoogleTest/GoogleMock framework for testing [6], with travis.ci continuous integration.

- Deterministic, finite-element-based transport code.
- Coded in C++, using the C++17 standard. A python script can automate creation of input files.
- Uses the deal.II finite-element library [4].
- Parallel processor (MPI) calculations are supported using PETSc [9, 8, 2].
- Uses the GoogleTest/GoogleMock framework for testing [6], with travis.ci continuous integration.
- Uses the Google Protocol Buffers file format for cross-sections.

• Supports 1-, 2-, and 3-D solves.

- Supports 1-, 2-, and 3-D solves.
- Two 2nd-order formulations of the transport equation implemented: diffusion and self-adjoint angular flux equation.

- Supports 1-, 2-, and 3-D solves.
- Two 2nd-order formulations of the transport equation implemented: diffusion and self-adjoint angular flux equation.
- Acceleration methods in development: nonlinear diffusion acceleration (NDA).

- Supports 1-, 2-, and 3-D solves.
- Two 2nd-order formulations of the transport equation implemented: diffusion and self-adjoint angular flux equation.
- Acceleration methods in development: nonlinear diffusion acceleration (NDA).
- Future methods: transport two-grid acceleration (TTG), and a combination of NDA and TTG.

- Supports 1-, 2-, and 3-D solves.
- Two 2nd-order formulations of the transport equation implemented: diffusion and self-adjoint angular flux equation.
- Acceleration methods in development: nonlinear diffusion acceleration (NDA).
- Future methods: transport two-grid acceleration (TTG), and a combination of NDA and TTG.
- Instrumentation in development: *in-situ* stepwise Fourier Analysis.

Design paradigm

Conclusion

Why acceleration methods?



Design paradigm

Conclusion

Why acceleration methods?

• Implementing and analyzing acceleration methods has practical challenges.

Conclusion

- Implementing and analyzing acceleration methods has practical challenges.
- We are developing a new code aimed at helping developers of new methods.

Conclusion

- Implementing and analyzing acceleration methods has practical challenges.
- We are developing a new code aimed at helping developers of new methods.
- We hope that the code will ease the burden of coding up new methods, and help provide good, useful data for understanding if and why the methods are worthwhile to implement in production level codes.

Thank you

References

[1] B. T. Adams and Jim E. Morel.

A Two-Grid Acceleration Scheme for the Multigroup Sn Equations with Neutron Upscattering.

Nuclear Science and Engineering, 115(May):253-264, 1993.

[2] Satish Balay, William D. Gropp, Lois Curfman McInnes, and Barry F. Smith.

Efficient management of parallelism in object oriented numerical software libraries.

In E. Arge, A. M. Bruaset, and H. P. Langtangen, editors, Modern Software Tools in Scientific Computing, pages 163–202.

Birkhäuser Press, 1997.

[3] E. E. Lewis and W.F. Miller, Jr.

Computational Methods of Neutron Transport.

American Nuclear Society, 1993.

[4] G. Alzetta et al.

The deal.II library, version 9.0.

Journal of Numerical Mathematics, 26(4):173-183, 2018.

[5] Thomas M. Evans, Kevin T. Clarno, and Jim E. Morel.

A Transport Acceleration Scheme for Multigroup Discrete Ordinates with Upscattering.

Nuclear Science and Engineering, 165:292-304, 2010.

[6] Google.

Googletest - Google Testing and Mocking Framework.

https://github.com/google/googletest.

Accessed: 2017 December 20.

[7] H. Park, D. A. Knoll, and C. K. Newman.

Nonlinear Acceleration of Transport Criticality Problems.

Nuclear Science and Engineering, 172(1):52-65, 2012.

[8] et al. Satish Balay.

PETSc users manual.

Technical Report ANL-95/11 - Revision 3.12, Argonne National Laboratory, 2019.

[9] et al. Satish Balay.

PETSc Web page.

https://www.mcs.anl.gov/petsc, 2019.

